Diethylmalonic acid, 3-bromobenzyl dodecyl ester

Inchi: InChI=1S/C26H41BrO4/c1-4-7-8-9-10-11-12-13-14-15-19-30-24(28)26(5-2,6-3)25(29)31-

InchiKey: DDXAZUIJVHZLLA-UHFFFAOYSA-N

Formula: C26H41BrO4

SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Br)c1

Mol. weight [g/mol]: 497.50

Physical Properties

Property code	Value	Unit	Source
gf	-179.86	kJ/mol	Joback Method
hf	-826.93	kJ/mol	Joback Method
hfus	60.19	kJ/mol	Joback Method
hvap	99.86	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	7.763		Crippen Method
mcvol	385.820	ml/mol	McGowan Method
pc	965.67	kPa	Joback Method
rinpol	3024.00		NIST Webbook
rinpol	3024.00		NIST Webbook
tb	1041.45	K	Joback Method
tc	1275.40	K	Joback Method
tf	628.26	K	Joback Method
vc	1.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1283.39	J/mol×K	1041.45	Joback Method
cpg	1299.48	J/mol×K	1080.44	Joback Method
cpg	1314.23	J/mol×K	1119.43	Joback Method
cpg	1327.74	J/mol×K	1158.42	Joback Method
cpg	1340.11	J/mol×K	1197.41	Joback Method
cpg	1351.44	J/mol×K	1236.41	Joback Method
cpg	1361.82	J/mol×K	1275.40	Joback Method
dvisc	0.0001582	Pa×s	628.26	Joback Method

dvisc	0.0000843	Pa×s	697.12	Joback Method
dvisc	0.0000503	Pa×s	765.99	Joback Method
dvisc	0.0000327	Pa×s	834.85	Joback Method
dvisc	0.0000227	Pa×s	903.72	Joback Method
dvisc	0.0000166	Pa×s	972.58	Joback Method
dvisc	0.0000126	Pa×s	1041.45	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368419&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume